

chain nodes :

14 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

12-14 13-16

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 5-11 6-13 7-8 8-9 9-10 11-12 12-13

exact/norm bonds :

2-7 3-10 5-11 6-13 7-8 8-9 9-10 11-12 12-13 12-14

exact bonds :

13-16

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:C,H,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:CLASS 16:CLASS

L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:203786 CAPLUS
 DN 140:243724
 ED Entered STN: 14 Mar 2004
 TI Cyclopenta[b]naphthalene derivatives
 IN Lietzau, Lars; Bremer, Matthias; Klasen-Memmer, Melanie; Heckmeier, Michael
 PA Merck Patent G.m.b.H., Germany
 SO PCT Int. Appl., 103 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 IC ICM C07C025-22
 ICS C07C022-08; C07C025-24; C07C043-225; C09K019-32
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 75

FAN.CNT 2

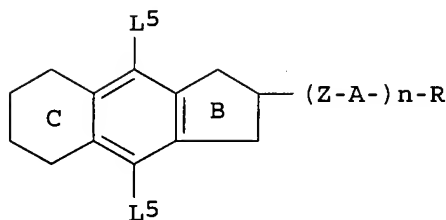
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	DE 10324843	A1	20041223	DE 2003-10324843	20030602
	AU 2003258538	A1	20040319	AU 2003-258538	20030728
	EP 1532090	A1	20050525	EP 2003-790821	20030728
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005537334	T	20051208	JP 2004-569707	20030728
	US 2006165915	A1	20060727	US 2005-524846	20050218
PRAI	DE 2002-10238999	A	20020826		
	DE 2003-10324843	A	20030602		
	WO 2003-EP8285	W	20030728		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004020375	ICM	C07C025-22
	ICS	C07C022-08; C07C025-24; C07C043-225; C09K019-32
	IPCI	C07C0025-22 [ICM,7]; C07C0022-08 [ICS,7]; C07C0022-00 [ICS,7,C*]; C07C0025-24 [ICS,7]; C07C0025-00 [ICS,7,C*]; C07C0043-225 [ICS,7]; C07C0043-00 [ICS,7,C*]; C09K0019-32 [ICS,7]
	IPCR	G02F0001-139 [I,A]; C07C0017-00 [I,C*]; C07C0017-093 [I,A]; C07C0017-25 [I,A]; C07C0017-35 [I,A]; C07C0017-354 [I,A]; C07C0022-00 [I,C*]; C07C0022-08 [I,A]; C07C0025-00 [I,C*]; C07C0025-22 [I,A]; C07C0025-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-46 [I,A]; C07C0045-64 [I,A]; C07C0049-00 [I,C*]; C07C0049-697 [I,A]; C07C0255-00 [I,C*]; C07C0255-52 [I,A]; C09K0019-32 [I,C*]; C09K0019-32 [I,A]; C09K0019-34 [I,C*]; C09K0019-34 [I,A]; C09K0019-54 [I,C*]; C09K0019-54 [I,A]; G02F0001-13 [I,C*]; G02F0001-13 [I,A]
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		C07C022/08; C07C025/22; C07C025/24; C07C045/46+49/697; C07C045/46+49/755; C07C045/64+49/747; C07C049/697; C07C255/52; C09K019/32; C09K019/34A
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	IPCR	C07C0017-00 [I,C*]; C07C0017-093 [I,A]; C07C0017-25 [I,A]; C07C0017-35 [I,A]; C07C0017-354 [I,A]; C07C0022-00 [I,C*]; C07C0022-08 [I,A]; C07C0025-00 [I,C*]; C07C0025-22 [I,A]; C07C0025-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-46 [I,A]; C07C0045-64 [I,A]; C07C0049-00 [I,C*]; C07C0049-697 [I,A]; C07C0255-00 [I,C*]; C07C0255-52 [I,A]; C09K0019-32 [I,A]; C09K0019-32 [I,C*]; C09K0019-34 [I,A]; C09K0019-34 [I,C*]
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 C09K0019-54 [I,C*]; C09K0019-54 [I,A]; G02F0001-13
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 NCL 428/001.100; 252/299.610; 252/299.620; 585/021.000
 ECLA C07C017/093+25/22; C07C017/25+25/22; C07C017/25+25/24;
 C07C017/35+25/22; C07C017/35+25/24; C07C017/354+25/22;
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 C07C045/46+49/755; C07C045/64+49/747; C07C049/697;
 C07C255/52; C09K019/32; C09K019/34A
 OS MARPAT 140:243724
 GI



AB The invention relates to cyclopenta[b]naphthalene derivs. of general
 formula I (C = 6-membered ring with substituents selected from H,
 C1-15-alkyl, alkoxy, etc.; B = 5-membered ring with substituents selected
 from H, C1-15-alkyl, alkoxy, etc.; Z = single bond, double bond, -CF2O-,
 -OCF2-, etc.; A = 1,4-phenylene, 1,4-cyclohexylene, etc.; R = H,
 C1-15-alkyl, alkoxy, etc.; L5, L6 = H, C1-15-alkyl, alkoxy, etc.; n =
 0-3), the use thereof in liquid crystal or mesogenous media, liquid crystal or
 mesogenous media comprising at least one of said cyclopenta[b]naphthalene

derivs. and electrooptical display elements comprising said liquid crystal or mesogenous media.

ST cyclopenta naphthalene synthesis liq crystal mesogenous media
electrooptical display

IT Liquid crystal displays
Liquid crystals

(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

IT 666732-85-0P 666732-87-2P 666732-89-4P

666732-91-8P 666732-93-0P 666732-95-2P 666732-97-4P

666732-99-6P 666733-01-3P 666733-03-5P 666733-05-7P 666733-07-9P

666733-09-1P 666733-11-5P 666733-13-7P

666733-15-9P 669005-43-0P 669005-44-1P 669005-45-2P

669005-46-3P 669005-47-4P 669005-48-5P 669005-49-6P 669005-50-9P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

IT 75-77-4, Chlorotrimethylsilane, reactions 100-39-0, Benzylbromide
540-63-6, 1,2-Ethanedithiol 7664-39-3, Hydrofluoric acid, reactions
7719-09-7, Thionylchloride 57848-46-1 64248-58-4 104089-16-9
107263-95-6, N-Fluoropyridinium triflate 610312-65-7 669005-29-2
669005-36-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

IT 13772-59-3P 666732-11-2P 666732-13-4P 666732-15-6P 666732-17-8P

666732-19-0P 666732-22-5P 666732-24-7P 666732-26-9P 666732-28-1P

666732-30-5P 666732-32-7P 666732-40-7P 666732-42-9P 666732-44-1P

666732-46-3P 666732-48-5P 666732-50-9P 666732-52-1P 666732-55-4P

666732-57-6P 666732-59-8P 666732-61-2P 666732-63-4P 666732-65-6P

666732-67-8P 666732-69-0P 666732-71-4P 666732-74-7P 666732-76-9P

666732-79-2P 666732-81-6P 666732-83-8P 669005-26-9P 669005-27-0P

669005-28-1P 669005-30-5P 669005-31-6P 669005-32-7P 669005-33-8P

669005-34-9P 669005-35-0P 669005-37-2P 669005-38-3P 669005-39-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

IT 669005-40-7P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Clariant International; EP 1223209 A 2002 CAPLUS

(2) Hoechst Ag; DE 4434974 A 1996 CAPLUS

(3) Merck Patent GmbH; WO 0246330 A 2002 CAPLUS

(4) Montell Technology Co; WO 9846547 A 1998 CAPLUS

(5) Yokokoji, O; JP 06263663 A 1994 CAPLUS

IT 666732-85-0P 666732-87-2P 666732-89-4P

666732-91-8P 666733-11-5P 666733-13-7P

666733-15-9P

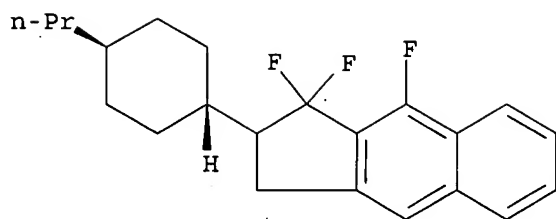
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal display)

RN 666732-85-0 CAPLUS

CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)-(9CI) (CA INDEX NAME)

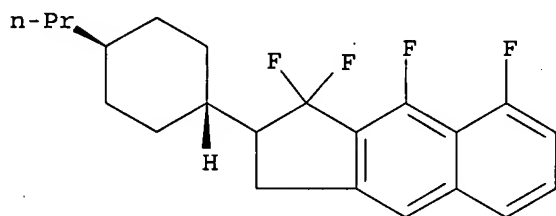
Relative stereochemistry.



RN 666732-87-2 CAPLUS

CN 1H-Benz[f]indene, 1,1,8,9-tetrafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

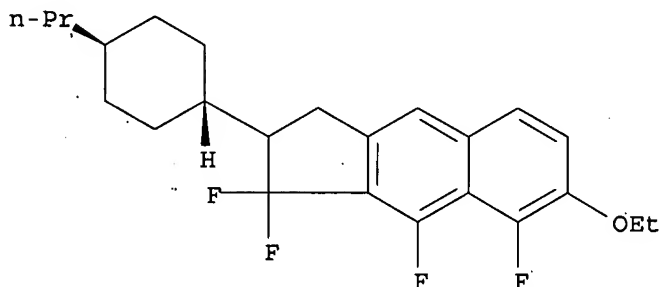
Relative stereochemistry.



RN 666732-89-4 CAPLUS

CN 1H-Benz[f]indene, 7-ethoxy-1,1,8,9-tetrafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

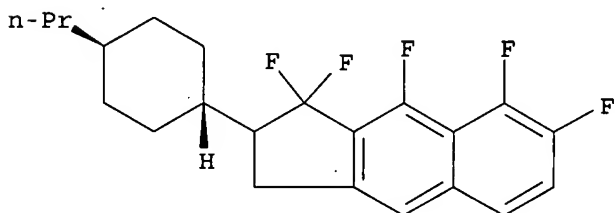
Relative stereochemistry.



RN 666732-91-8 CAPLUS

CN 1H-Benz[f]indene, 1,1,7,8,9-pentafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

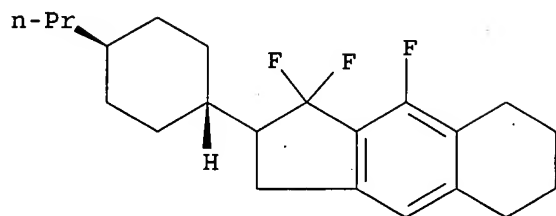
Relative stereochemistry.



RN 666733-11-5 CAPLUS

CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

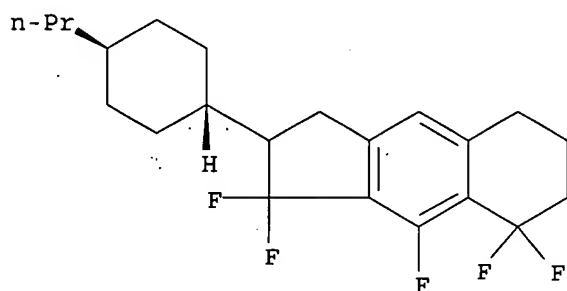
Relative stereochemistry.



RN 666733-13-7 CAPLUS

CN 1H-Benz[f]indene, 1,1,8,8,9-pentafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

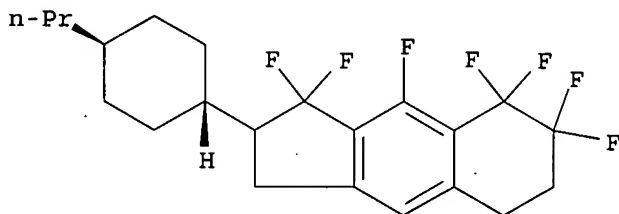
Relative stereochemistry.



RN 666733-15-9 CAPLUS

CN 1H-Benz[f]indene, 1,1,7,7,8,8,9-heptafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:177941 CAPLUS

DN 140:225895

ED Entered STN: 04 Mar 2004

TI Cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display

IN Lietzau, Lars; Bremer, Matthias; Klasen-Memmer, Melanie

PA Merck Patent G.m.b.H., Germany

SO Ger. Offen., 46 pp.

CODEN: GWXXBX

DT Patent

LA German

IC ICM C07C025-22

ICS C07C043-225; C07C049-697; C07D319-06; C09K019-32; C09K019-34;

G02F001-137; G09F009-35; C07C069-00; C07C323-00; C07C255-00;

C07C331-00

CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other

Reprographic Processes)

Section cross-reference(s): 75

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10238999	A1	20040304	DE 2002-10238999	20020826
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	EP 1532090	A1	20050525	EP 2003-790821	20030728
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	JP 2005537334	T	20051208	JP 2004-569707	20030728
	US 2006165915	A1	20060727	US 2005-524846	20050218
PRAI	DE 2002-10238999	A	20020826		
	DE 2003-10324843	A	20030602		
	WO 2003-EP8285	W	20030728		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
DE 10238999	ICM	C07C025-22
	ICS	C07C043-225; C07C049-697; C07D319-06; C09K019-32; C09K019-34; G02F001-137; G09F009-35; C07C069-00; C07C323-00; C07C255-00; C07C331-00
	IPCI	C07C0025-22 [ICM,7]; C07C0025-00 [ICM,7,C*]; C07C0043-225 [ICS,7]; C07C0043-00 [ICS,7,C*]; C07C0049-697 [ICS,7]; C07C0049-00 [ICS,7,C*]; C07D0319-06 [ICS,7]; C07D0319-00 [ICS,7,C*]; C09K0019-32 [ICS,7]; C09K0019-34 [ICS,7]; G02F0001-137 [ICS,7]; G02F0001-13 [ICS,7,C*]; G09F0009-35 [ICS,7]; C07C0069-00 [ICS,7]; C07C0323-00 [ICS,7]; C07C0255-00 [ICS,7]; C07C0331-00 [ICS,7]
	IPCR	C07C0017-00 [I,C*]; C07C0017-093 [I,A]; C07C0017-25 [I,A]; C07C0017-35 [I,A]; C07C0017-354 [I,A]; C07C0022-00 [I,C*]; C07C0022-08 [I,A]; C07C0025-00 [I,C*]; C07C0025-22 [I,A]; C07C0025-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-46 [I,A]; C07C0045-64 [I,A]; C07C0049-00 [I,C*]; C07C0049-697 [I,A]; C07C0255-00 [I,C*]; C07C0255-52 [I,A]; C09K0019-32 [I,A]; C09K0019-32 [I,C*]; C09K0019-34 [I,A]; C09K0019-34 [I,C*]
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WO 2004020375	IPCI	C07C0025-22 [ICM,7]; C07C0022-08 [ICS,7]; C07C0022-00 [ICS,7,C*]; C07C0025-24 [ICS,7]; C07C0025-00 [ICS,7,C*]; C07C0043-225 [ICS,7]; C07C0043-00 [ICS,7,C*]; C09K0019-32 [ICS,7]
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C07C0025-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-46 [I,A]; C07C0045-64 [I,A]; C07C0049-00 [I,C*]; C07C0049-697 [I,A]; C07C0255-00 [I,C*]; C07C0255-52 [I,A]; C09K0019-32 [I,C*]; C09K0019-32 [I,A]; C09K0019-34 [I,C*]; C09K0019-34 [I,A]; C09K0019-54 [I,C*]; C09K0019-54 [I,A]; G02F0001-13 [I,C*]; G02F0001-13 [I,A]

AU 2003258538 ECLA C07C017/093+25/22; C07C017/25+25/22; C07C017/25+25/24; C07C017/35+25/22; C07C017/35+25/24; C07C017/354+25/22; C07C022/08; C07C025/22; C07C025/24; C07C045/46+49/697; C07C045/46+49/755; C07C045/64+49/747; C07C049/697; C07C255/52; C09K019/32; C09K019/34A

AU 2003258538 IPCI C07C0025-22 [ICM,7]; C07C0043-225 [ICS,7]; C07C0043-00 [ICS,7,C*]; C09K0019-32 [ICS,7]; C07C0022-08 [ICS,7]; C07C0022-00 [ICS,7,C*]; C07C0025-24 [ICS,7]; C07C0025-00 [ICS,7,C*]

AU 2003258538 IPCR G02F0001-139 [I,A]; C07C0017-00 [I,C*]; C07C0017-093 [I,A]; C07C0017-25 [I,A]; C07C0017-35 [I,A]; C07C0017-354 [I,A]; C07C0022-00 [I,C*]; C07C0022-08 [I,A]; C07C0025-00 [I,C*]; C07C0025-22 [I,A]; C07C0025-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-46 [I,A]; C07C0045-64 [I,A]; C07C0049-00 [I,C*]; C07C0049-697 [I,A]; C07C0255-00 [I,C*]; C07C0255-52 [I,A]; C09K0019-32 [I,C*]; C09K0019-32 [I,A]; C09K0019-34 [I,C*]; C09K0019-34 [I,A]; C09K0019-54 [I,C*]; C09K0019-54 [I,A]; G02F0001-13 [I,C*]; G02F0001-13 [I,A]

EP 1532090 IPCI C07C0025-22 [ICM,7]; C07C0022-08 [ICS,7]; C07C0022-00 [ICS,7,C*]; C07C0025-00 [ICS,7]; C07C0025-24 [ICS,7]

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JP 2005537334 IPCI C07C0025-22 [ICM,7]; C07C0025-00 [ICM,7,C*]; C09K0019-32 [ICS,7]; C09K0019-54 [ICS,7]; G02F0001-13 [ICS,7]; G02F0001-139 [ICS,7]

JP 2005537334 FTERM 2H088/JA10; 2H088/KA27; 4H006/AA01; 4H006/AA03; 4H006/AB64; 4H027/BC05; 4H027/BD10; 4H027/BD11; 4H027/BE05; 4H027/DM00; 4H027/DM01; 4H027/DM03; 4H027/DM05

US 2006165915 IPCI C09K0019-32 [I,A]; C09K0019-34 [I,A]; C07C0013-54 [I,A]; C07C0013-547 [I,A]; C07C0013-00 [I,C*]

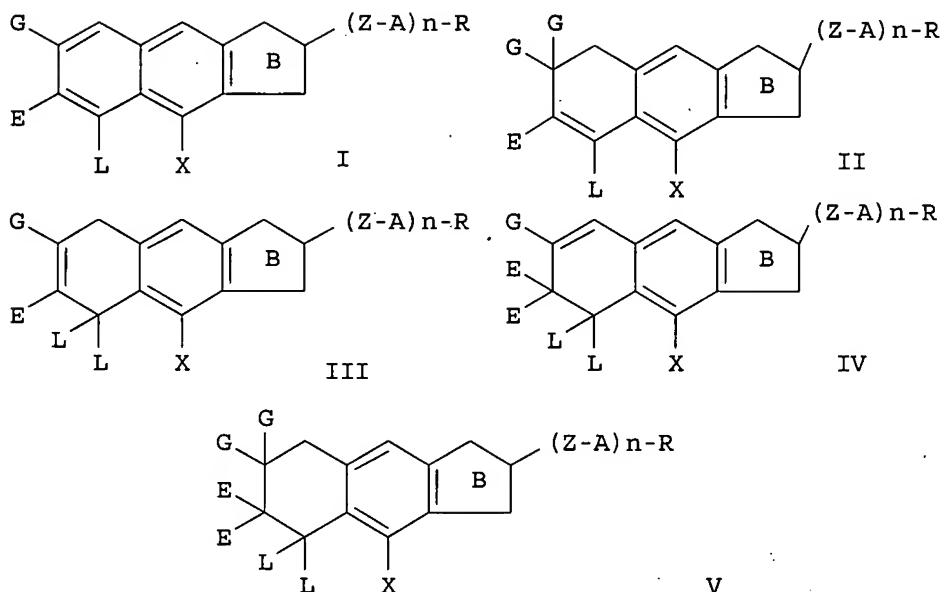
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US 2006165915 NCL 428/001.100; 252/299.610; 252/299.620; 585/021.000

US 2006165915 ECLA C07C017/093+25/22; C07C017/25+25/22; C07C017/25+25/24; C07C017/35+25/22; C07C017/35+25/24; C07C017/354+25/22;

C07C022/08; C07C025/22; C07C025/24; C07C045/46+49/697;
 C07C045/46+49/755; C07C045/64+49/747; C07C049/697;
 C07C255/52; C09K019/32; C09K019/34A

OS MARPAT 140:225895
 GI



- AB The title cyclopenta[b]naphthalene derivative having a neg. $\Delta\epsilon$ is represented by general formula I, II, III, IV and V (B = five membered ring with F-substituent; A = 1,4-phenylene, etc.; Z = single bond, double bond, -CF₂O-, etc.; R = H, C1-15-alkyl, alkoxy, etc.; X, L = H, C1-15-alkyl, etc.; E, G = H, C1-15-alkyl, etc.; n = 0-3). The cyclopenta[b]naphthalene derivs. are synthesized.
- ST nematic liq crystal mixt display cyclopenta naphthalene prepn
- IT Liquid crystal displays
 (cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)
- IT Liquid crystals
 (nematic; cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)
- IT 666732-85-0P 666732-87-2P 666732-89-4P
 666732-91-8P 666732-93-0P 666732-95-2P 666732-97-4P
 666732-99-6P 666733-01-3P 666733-03-5P 666733-05-7P 666733-07-9P
 666733-09-1P 666733-11-5P 666733-13-7P
 666733-15-9P
- RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)
- IT 75-77-4, Chlorotrimethylsilane, reactions 77-48-5, 1,3-Dibromo-5,5-dimethylhydantoin 100-39-0 109-80-8, 1,3-Propanedithiol 540-63-6, 1,2-Ethanedithiol 7664-39-3, Hydrogen fluoride, reactions 57848-46-1 104089-16-9 107263-95-6, N-Fluoropyridinium triflate 610312-65-7
- RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)
- IT 13772-59-3P 666732-11-2P 666732-13-4P 666732-15-6P 666732-17-8P
 666732-19-0P 666732-22-5P 666732-24-7P 666732-26-9P 666732-28-1P

666732-30-5P 666732-32-7P 666732-36-1P 666732-38-3P 666732-40-7P
 666732-42-9P 666732-44-1P 666732-46-3P 666732-48-5P 666732-50-9P
 666732-52-1P 666732-55-4P 666732-57-6P 666732-59-8P 666732-61-2P
 666732-63-4P 666732-65-6P 666732-67-8P 666732-69-0P 666732-71-4P
 666732-74-7P 666732-76-9P 666732-79-2P 666732-81-6P 666732-83-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT 666732-85-0P 666732-87-2P 666732-89-4P
 666732-91-8P 666733-11-5P 666733-13-7P
 666733-15-9P

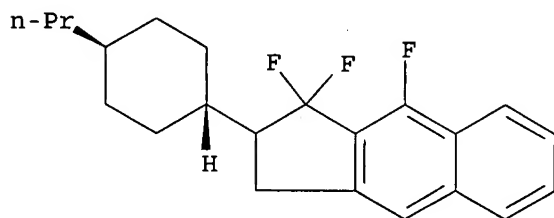
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

RN 666732-85-0 CAPLUS

CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

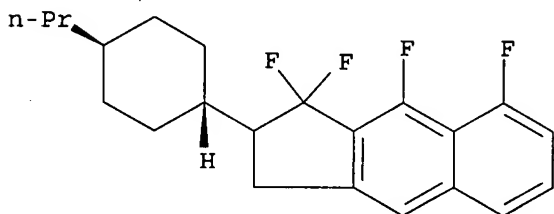
Relative stereochemistry.



RN 666732-87-2 CAPLUS

CN 1H-Benz[f]indene, 1,1,8,9-tetrafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

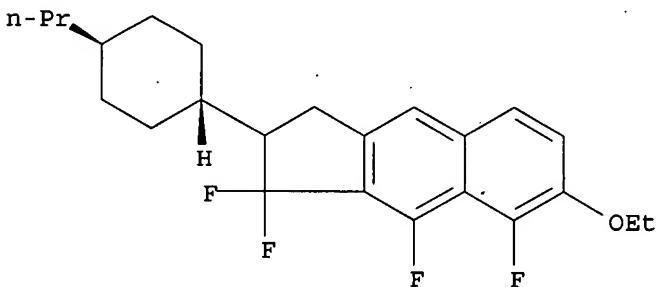
Relative stereochemistry.



RN 666732-89-4 CAPLUS

CN 1H-Benz[f]indene, 7-ethoxy-1,1,8,9-tetrafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

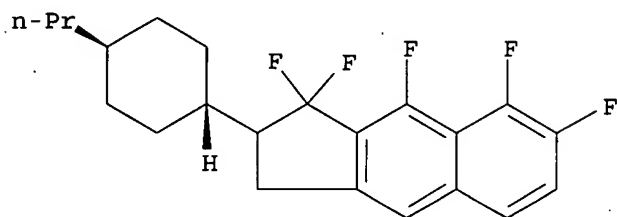
Relative stereochemistry.



RN 666732-91-8 CAPLUS

CN 1H-Benz[f]indene, 1,1,7,8,9-pentafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

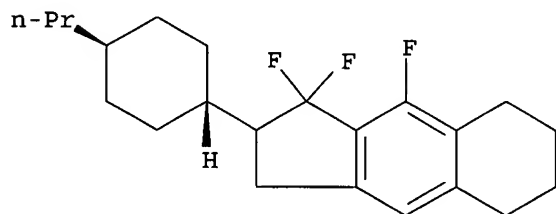
Relative stereochemistry.



RN 666733-11-5 CAPLUS

CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

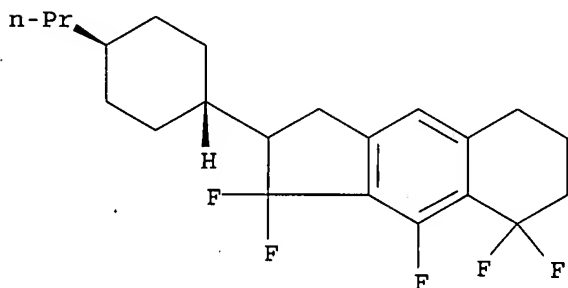
Relative stereochemistry.



RN 666733-13-7 CAPLUS

CN 1H-Benz[f]indene, 1,1,8,8,9-pentafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

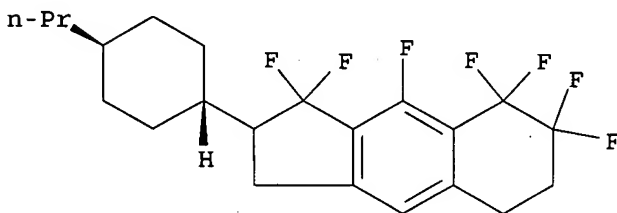
Relative stereochemistry.



RN 666733-15-9 CAPLUS

CN 1H-Benz[f]indene, 1,1,7,7,8,8,9-heptafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2002:817619 CAPLUS
 DN 138:237618
 ED Entered STN: 28 Oct 2002
 TI MNDO Study of the (Anti)aromaticity of Fluorine-Containing
 Cyclopentadienyl, Indenyl, and Cyclopenta[b]naphthyl Cations
 AU Shchegoleva, L. N.; Karpov, V. M.; Platonov, V. E.
 CS Siberian Division, Vorozhtsov Novosibirsk Institute of Organic Chemistry,
 Russian Academy of Sciences, Novosibirsk, 630090, Russia
 SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi
 Khimii) (2002), 38(7), 995-1000
 CODEN: RJOCEQ; ISSN: 1070-4280
 PB MAIK Nauka/Interperiodica Publishing
 DT Journal
 LA English
 CC 22-2 (Physical Organic Chemistry)
 AB MNDO calcns. were performed to estimate the aromaticity (antiaromaticity) of
 F-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations in
 terms of the Dewar-Breslow criterion which uses the difference in the
 enthalpies of formation of isomeric cations with closed and open
 π -systems as aromaticity index. The aromaticity is strongly determined by
 both the structure of the C skeleton and the number and position of F atoms.
 A linear correlation was revealed between the aromaticity index and the
 energy of the lowest singlet-singlet excitation for cations having a
 cyclic π -system.
 ST MNDO aromaticity antiaromaticity fluorine cyclopentadienyl indenyl
 cyclopentanaphthyl cation
 IT Linear free energy relationship
 (Dewar-Breslow aromaticity index vs. singlet excitation; MNDO study of
 (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and
 cyclopenta[b]naphthyl cations)
 IT Antiaromaticity
 Aromaticity
 Correlation analysis
 Formation enthalpy
 Frontier molecular orbital
 HOMO (molecular orbital)
 Jahn-Teller effect
 LUMO (molecular orbital)
 MNDO
 Singlet state excitation
 Substituent effects
 (MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl,
 indenyl, and cyclopenta[b]naphthyl cations)
 IT Carbocations
 RL: PRP (Properties)
 (MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl,
 indenyl, and cyclopenta[b]naphthyl cations)
 IT Indexes
 (aromaticity; MNDO study of (anti)aromaticity of fluorine-containing
 cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)
 IT Isomers
 (cation; MNDO study of (anti)aromaticity of fluorine-containing
 cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)
 IT 49762-89-2 58741-78-9 62302-99-2 128654-07-9 192275-45-9
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 192275-51-7 214264-89-8 240136-11-2 501370-81-6 501370-82-7
 501370-83-8 501370-84-9 501370-85-0 501370-87-2 501370-88-3
 501370-89-4 501370-90-7 501370-91-8 501370-92-9
 501370-93-0
 RL: PRP (Properties)
 (MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl,
 indenyl, and cyclopenta[b]naphthyl cations)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
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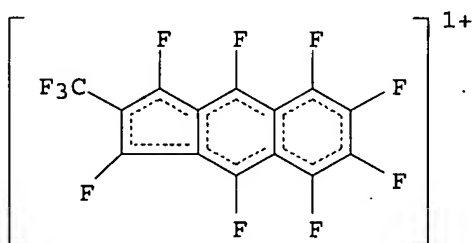
IT 501370-90-7 501370-91-8

RL: PRP (Properties)

(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)

RN 501370-90-7 CAPLUS

CN Benz[f]indenyl, 1,3,4,5,6,7,8,9-octafluoro-2-(trifluoromethyl)- (9CI)
(CA INDEX NAME)



RN 501370-91-8 CAPLUS

CN Benz[f]indenyl, 1,3,4,5,8,9-hexafluoro-2-(trifluoromethyl)- (9CI) (CA
INDEX NAME)

